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Photophysics of single-walled carbon nanotubes: similarity with π-conjugated polymer[1]

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Coulomb electron-electron (e-e) interactions among the π-electrons have a strong effect on the energy spectra of semiconducting single-walled carbon nanotubes (S-SWCNTs), because of their quasi-one-dimensionality. The primary photoexcitations in S-SWCNTs as a consequence of e-e interactions are excitons, as opposed to free electrons and holes. There already exists a vast literature on excitons in π-conjugated polymers, the other class of carbon-based quasi-one-dimensional semiconductors. In order to seek guidance from this knowledge base, we have performed theoretical calculations of the excited state electronic structures, linear absorptions and excited state absorptions for ten different S-SWCNTs with a wide range in diameters, [2] within the same correlated π-electron model that has previously been applied to π-conjugated polymers. We found remarkable similarities in the excitonic energy spectra and nonlinear optical properties of S-SWCNTs on the one hand, and π-conjugated polymers on the other. The "essential states" model [3] of third-order optical nonlinearity, previously developed for π-conjugated polymers, applies also to S-SWCNTs (with minor modifications for chiral S-SWCNTs which lack center of inversion). Our theory is able to explain semiquantitatively the results of nonlinear spectroscopic measurements on both S-SWCNTs and π-conjugated polymers. For wide S-SWCNTs with diameters ranging from 0.8–1.0 nm, we calculate exciton binding energies of 0.3–0.4 eV, in strong agreement with the values predicted from the experiments. We also remark on the occurrence of dark excitons below the optical excitons in the S-SWCNTs, [4] and the consequence thereof on the photoluminescence of these materials.

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[2]H. Zhao, *et al.*, cond-mat/0506097; J. W. Kennedy, *et al.*, cond-mat/0505071.
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[4]H. Zhao and S. Mazumdar, Phys. Rev. Lett. **93**, 157402 (2004).